The MFA ground states for the extended Bose-Hubbard model with a three-body constraint

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Abstract

We address the intensively studied extended bosonic Hubbard model (EBHM) with truncation of the on-site Hilbert space to the three lowest occupation states $n = 0, 1, 2$ in frames of the $S = 1$ pseudospin formalism. Similar model was recently proposed to describe the charge degree of freedom in a model high-T_c cuprate with the on-site Hilbert space reduced to the three effective valence centers, nominally $Cu^{1+;2+;3+}$. With small corrections the model becomes equivalent to a strongly anisotropic $S = 1$ quantum magnet in an external magnetic field. We have applied a generalized mean-field approach and quantum Monte-Carlo technique for the model 2D $S = 1$ system with a two-particle transport to find the ground state phase with its evolution under deviation from half-filling.

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1. Introduction

These days spin algebra and spin Hamiltonians are used not only in the traditional fields of spin magnetism but in so-called pseudospin lattice systems with the on-site occupation constraint. For instance, the $S = 1$ pseudospin formalism was applied to study an extended Bose-Hubbard model (EHBM) with truncation of the on-site Hilbert space to the three lowest occupation states $n = 0, 1, 2$ (semi-hard-core bosons) considered to be three pseudospin states with $M = -1$, $M = 0$, $M = +1$, respectively (see [1] and references therein). At variance with quantum $s = 1/2$ systems the Hamiltonian of $S = 1$ spin lattices in general is characterized by several additional terms such as a single ion anisotropy that results in their rich phase diagrams. Recently we made use of the $S = 1$ pseudospin formalism to describe the charge degree of freedom in high-T_c cuprates with the on-site Hilbert space reduced to only the three effective valence centers $[CuO_4]^{7-,6-,5-}$ (nominally $Cu^{1+;2+;3+}$) [2, 3, 4, 5].

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2. $S = 1$ (pseudo)spin Hamiltonian

The $S = 1$ spin algebra includes the eight nontrivial independent spin operators: spin-dipole moment $\mathbf{S}$ and five spin-quadrupole operators $Q_{ij} = (\frac{1}{2}\{S_i, S_j\} - \frac{2}{3}\delta_{ij})$ whose mean values define so-called spin-nematic order. Spin operators $S_\pm$ and $T_\pm = \{S_z, S_\pm\}$ change the pseudospin projection (and occupation number) by ± 1, while $S_\pm^2$ changes the pseudospin projection by ± 2.

Hereafter in the paper we will focus on a simplified 2D $S = 1$ (pseudo)spin Hamiltonian with the nearest neighbor coupling and the only two-particle transport term (inter-site biquadratic anisotropy) as follows:

$$\hat{H} = \sum_i (\Delta S_{iz}^2 - \mu S_{iz}) + V \sum_{\langle ij \rangle} S_{iz} S_{jz} - t \sum_{\langle ij \rangle} (S_{i+}^2 S_{j-}^2 + S_{i-}^2 S_{j+}^2), \qquad (1)$$

where $V > 0$, $t > 0$. The first single-site term in $\hat{H}$ describes the effects of a bare pseudo-spin splitting and relates with the on-site density-density interactions, or correlations: $\Delta = U/2$. The second term, or a pseudospin Zeeman coupling may be related with a pseudo-magnetic field $\| Z$ which acts as analog of chemical potential μ for doped charge with a charge constraint:

$$\sum_i \langle S_{iz} \rangle = nN, \qquad (2)$$

where fixed n is the doped charge density. The third (Ising) term in $\hat{H}$ describes the effects of the short- and long-range inter-site density-density interactions. The last term in $\hat{H}$ describes the two-particle inter-site hopping. In the strong on-site attraction limit of the model (large easy-axis pseudospin on-site anisotropy) we arrive at the Hamiltonian of the hard-core, or local, bosons which was earlier considered to be a starting point for explanation of the cuprate high-T_c superconductivity [6]. The spin counterpart of $\hat{H}$ corresponds to an anisotropic $S = 1$ magnet with a single ion (on-site) and two-ion (bilinear and biquadratic) symmetric anisotropy in an external magnetic field. It describes an interplay of the Zeeman, single-ion and two-ion anisotropic terms giving rise to a competition of an (anti)ferromagnetic order along Z-axis with an in-plane XY spin-nematic order. A remarkable feature of the Hamiltonian (1) is that the on-site pseudospin states $M = 0$ and $|M| = 1$ do not mix under the inter-site coupling. The model allows us to directly study a continuous transformation of the semi-hard-core bosons to the effective hard-core bosons formed by boson pairs under driving the correlation parameter $\Delta = U/2$ to large negative values ("negative-U model"). The simplified model can be directly applied to a description of bosonic systems with suppressed one-particle hopping.

3. Mean-field approximation

To analyze the simplified model we start with a mean-field approximation (MFA) for 2D square lattice, however, at variance with a conventional classical

	ε	$\cos\theta_j$	$\cos\phi_j$
SF	$\delta-1+n^2(2\nu+1)$	-1	n
SS	$\delta-2\nu+2\lvert n\rvert\sqrt{4\nu^2-1}$	-1	$n+(-1)^j ab$
CO1	$\lvert n\rvert\,\delta$	$1-2\lvert n\rvert+2(-1)^j n$	σ
CO2	$(1-\lvert n\rvert)\,\delta+4\left(\lvert n\rvert-\frac{1}{2}\right)\nu$	$-1+2\lvert n\rvert+2(-1)^j n$	$(-1)^{j+1}$
CO3	$\lvert n\rvert\delta+4\left(\lvert n\rvert-\frac{1}{2}\right)\nu$	$1-2\lvert n\rvert+2(-1)^j\sigma\big(1-\lvert n\rvert\big)$	σ

Table 1: The energies and parameters of MFA GS phases. The index j is 0(1) for A(B) sublattice. The details of notations see in the text.

MFA we made use of more correct approach that takes into account the quantum nature of the $S=1$ (pseudo)spin states [7]. First we introduce a set of the on-site $S=1$ coherent states

$$|\mathbf{c}\rangle = c_{-1}|-1\rangle + c_0|0\rangle + c_{+1}|+1\rangle, \tag{3}$$

where the c_M coefficients can be represented as follows

$$c_1{=}\sin\frac{\theta}{2}\cos\frac{\phi}{2}e^{-i\frac{\alpha}{2}}, \quad c_0{=}\cos\frac{\theta}{2}e^{i\frac{\beta}{2}}, \quad c_{-1}{=}\sin\frac{\theta}{2}\sin\frac{\phi}{2}e^{i\frac{\alpha}{2}} \tag{4}$$

with θ, ϕ, α, β to be parameters defined by the minimization of the energy. The MFA energy can be written as follows

$$\begin{aligned} E \;=\; & \frac{\Delta}{2}\sum_i\Big(1-\cos\theta_i\Big)+\frac{V}{4}\sum_{\langle ij\rangle}\Big(1-\cos\theta_i\Big)\Big(1-\cos\theta_j\Big)\cos\phi_i\,\cos\phi_j - \\ & -\frac{t}{8}\sum_{\langle ij\rangle}\Big(1-\cos\theta_i\Big)\Big(1-\cos\theta_j\Big)\sin\phi_i\,\sin\phi_j\,\cos(\alpha_i-\alpha_j) - \\ & -\frac{\mu}{2}\sum_i\Big(1-\cos\theta_i\Big)\cos\phi_i. \end{aligned} \tag{5}$$

Here, the term with the chemical potential μ takes into account the constraint (2). It is worth noting that due to the absence of the one-particle inter-site hopping terms in Hamiltonian (1) the energy does not depend on phase parameter β, so the β remains undetermined.

In a two-sublattice A-B model, we arrive at the five MFA uniform phases for the ground state (GS). The energies and parameters of solutions are listed in Table.1. We use the notations: $\varepsilon = E/(tN)$, $\delta = \Delta/t$, $\nu = V/t$, $\sigma = \operatorname{sgn} n$, $a = \sqrt{\sqrt{\frac{2\nu+1}{2\nu-1}}-|n|}$, $b = \sqrt{\sqrt{\frac{2\nu-1}{2\nu+1}}-|n|}$. In all phases, the value of chemical potential μ satisfies the regular expression $\mu = t\,\partial\varepsilon/\partial n$. The solutions for SF and SS phases imply that $\alpha_A - \alpha_B = 0$ or π, in other phases this difference remains undefined.

	$\langle S_z\rangle_j$	$\langle P_0\rangle_j$	$\langle S^2_\pm\rangle_j$
SF	n	0	$\frac{\eta}{2}\sqrt{1-n^2}\,e^{\pm i\alpha}$
SS	$n+(-1)^j ab$	0	$\frac{\eta}{2}\big(a-(-1)^j\sigma\, b\big)\sqrt{\vert n\vert}\,e^{\pm i\alpha}$
CO1	$n-(-1)^j\vert n\vert$	$1-\vert n\vert+(-1)^j n$	0
CO2	$n-(-1)^j\big(1-\vert n\vert\big)$	$\vert n\vert+(-1)^j n$	0
CO3	$n-(-1)^j\big(1-\vert n\vert\big)$	$\big(1-\vert n\vert\big)\big(1+(-1)^j\sigma\big)$	0

Table 2: The order parameters of GS MFA phases. The index j is 0(1) for A(B) sublattice. Here $\eta=\pm1$ and the phase α remains undefined. Other details of notations see in the text.

The GS MFA phases differ by local charge density $\langle S_z\rangle$ and local density of $M=0$ (Cu^{2+}) states $\langle P_0\rangle = 1-\langle S_z^2\rangle$:

$$\langle S_z\rangle = \frac{1}{2}\,(1-\cos\theta)\cos\phi, \quad \langle P_0\rangle = \frac{1}{2}\,(1+\cos\theta)\,, \tag{6}$$

and by local superfluid order parameter, or pseudospin nematic order $\langle S^2_\pm\rangle$:

$$\big\langle S^2_\pm\big\rangle = \frac{1}{4}\,(1-\cos\theta)\sin\phi\; e^{\pm i\alpha}. \tag{7}$$

The density of superfluid component is related to helicity modulus [8]. This allow us to find an expression of the superfluid density ρ in terms of local superfluid order parameters in the two-sublattice MFA:

$$\rho = \mathrm{Re}\,\big(\,\big\langle S^2_{A+}\big\rangle\big\langle S^2_{B-}\big\rangle\,\big). \tag{8}$$

The local order parameters for the GS MFA phases are listed in Table.2.

Bose superfluid (SF) and supersolid (SS) phases are completely analogous to phases of charged hard-core bosons [6, 9] as these phases have no the $M=0$ states. The superfluid density in SF phase, $\rho=(1-n^2)/4$, has maximum value at $n=0$ and does not depend on inter-site density-density interactions parameter ν. In SS phase, the superfluid density $\rho=|n|/(2\sqrt{4\nu^2-1})$ decreases with rising of ν. The charge density differs on sublattices in SS phase and this phase becomes the pure charge-ordered one at $n=0$.

Stability conditions for SF phase

$$\delta<2, \quad n^2>\frac{2\nu-1}{2\nu+1}, \tag{9}$$

and for SS phase

$$\delta<2, \quad \nu>\frac{1}{2}, \quad \sqrt{\frac{2\nu-1}{2\nu+1}}-\frac{\big(1-\frac{\delta}{2}\big)^2}{\delta\sqrt{4\nu^2-1}}<|n|<\sqrt{\frac{2\nu-1}{2\nu+1}}, \tag{10}$$

define the boundary expression for SF and SS phases: $n^2 = (2\nu-1)/(2\nu+1)$. As the energies of SF and SS phases have the same dependence on the correlation parameter δ (see Table 1), the line of the SF-SS transition does not change with δ.

Three charge ordered MFA phases with $\left\langle S^2_{A,B\pm}\right\rangle = 0$ but different types of the sublattice occupation emerge if $\delta > 0$ and completely displace the superfluid phases at $\delta > 2$.

Stability conditions for the charge ordered 1 (CO1) are given by inequality

$$|n| < \min\left\{\frac{1}{2},\, \frac{\delta}{4\nu}\right\}. \tag{11}$$

Given $n = 0$ the CO1 phase consists of $M = 0$ centers. The striking feature of the CO1 phase is the independence of energy on inter-site interaction parameter ν. According to the two sublattices mean field approach, upon doping only one of the sublattices begins to be filled by $M = \pm 1$ centers depending on the sign of n. Numerical simulations with classical Monte-Carlo show that there is no difference in the sublattices occupations while $|n| \ll 1/2$, but this difference arises at $|n| \to 1/2$ according to the MFA expressions for $\langle S_z\rangle_j$ and $\langle P_0\rangle_j$.

Charge ordered 2 (CO2) phase has the stability conditions given by the expression

$$|n| < \min\left\{\frac{1}{2},\, 1 - \frac{\delta}{4\nu},\, \frac{8\delta\nu - \delta^2 - 4}{8|1-\delta\nu|}\right\}. \tag{12}$$

At $n = 0$, the CO2 phase is fully polarized, and with a deviation from $n = 0$ one of the sublattices is filled by $M = 0$ centers that leads to reducing of its $|\langle S_z\rangle|$.

The line of the CO1-CO2 transition for all $|n| < 1/2$ is defined by the expression $\delta = 2\nu$ that follows from the equality of energies of these phases.

Given $|n| = 1/2$ the parameters of CO1 and CO2 phases become equal to that of the charge ordered 3 (CO3) phase. Stability conditions of the CO3 phase are given by

$$\frac{1}{2} < |n| < \min\left\{1,\, \frac{8\delta\nu + \delta^2 + 4}{8(1+\delta\nu)}\right\}. \tag{13}$$

For the CO3 phase at $n = 1/2$, one of the sublattices is completely filled with $M = 1$ or $M = -1$ centers depending on the sign of n, while the second is completely filled by $M = 0$ centers. With the $|n|$ rising, the second sublattice is also filled by $|M| = 1$ centers.

Interestingly, all the local order parameters do not depend on the correlation parameter Δ, while this parameter governs the energy of different phases. Taking into account the on-site correlations and the stability conditions (9–13) we arrive at very rich and intricate phase diagrams for the model system as compared with relatively simple phase diagrams for hard-core bosons [6, 9]. The kind of transition between the GS phases is determined by the limiting values of the order parameters (see Table 2) on the transition lines. The SF-SS transition does not lead to discontinuities of the order parameters (the transition of the second kind) except the jump of the local superfluid order parameter

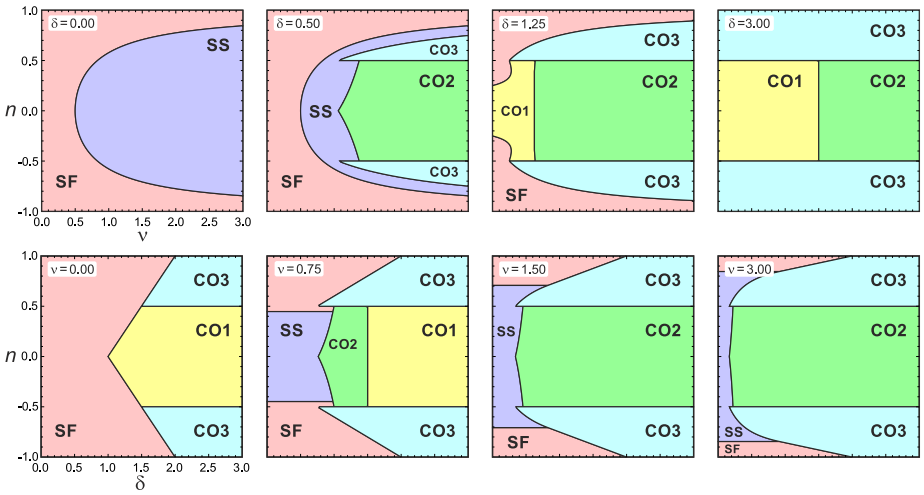

Figure 1: (Color online) The MFA GS phase diagrams for the inter-site interaction parameter ν variation (upper panels) and for the on-site correlation parameter δ variation (lower panels).

$\langle S^2_{\pm}\rangle$ at $n = 0$ (the point of the first kind transition). The CO1-CO3 and CO2-CO3 transitions at $n = 1/2$ are also continuous (of the second kind). All other transitions are discontinuous (of the first kind).

In Fig. 1 (upper panels) we show the MFA GS phase diagrams for the inter-site interaction parameter ν variation and for the on-site correlation parameter δ variation (lower panels). For $\delta = 0$, the phase diagram is the same as for hc-bosons [6]. With increasing δ, superfluid phases are rapidly replaced with the charge ordered phases. The replacement of the SS phase begins at $\delta > 0$ in the region of large values of the parameter ν. SS phase disappears completely when $\delta \approx 1.15$. For $\delta > 1$, in the region of small values of the parameter ν, the CO1 phase appears, which begins to displace the SF phase. This process begins at $n = 0$, where the value of the density of the superfluid component is maximal. For $\delta \geq 2$, the SF phase is completely replaced with the charge ordered phases.

Evolution with a change in the parameter ν also shows a rapid decrease in the fraction of superfluid phases on the phase diagram in comparison with the charge ordered phases. The most complicated phase diagram is observed for $\delta \approx 1.1$, $\nu \approx 0.65$ where the competition of the on-site and intersite interactions manifests itself most strongly. At half-filling $n = 0$ the positive values of the correlation parameter δ stabilize a limiting CO1 phase with $\langle S_{A,Bz}\rangle = \langle S^2_{A,Bz}\rangle = 0$, or a "parent Cu^{2+} phase" for a model cuprate, while positive values of ν stabilize a limiting CO2 phase with $\langle S_{A,Bz}\rangle = \pm 1$; $\langle S^2_{A,Bz}\rangle = 1$, or a checkerboard "antiferromagnetic" order of pseudospins along z-axis, or a disproportionated Cu^{1+}-Cu^{3+} phase for a model cuprate. As a result of the competition between the on-site and inter-site correlations we arrive at a "starting" CO1 phase for $\delta > 2\,\nu$ or CO2 phase for $\delta \leq 2\,\nu$. At $n = 0.5$ we see a transformation of the CO1

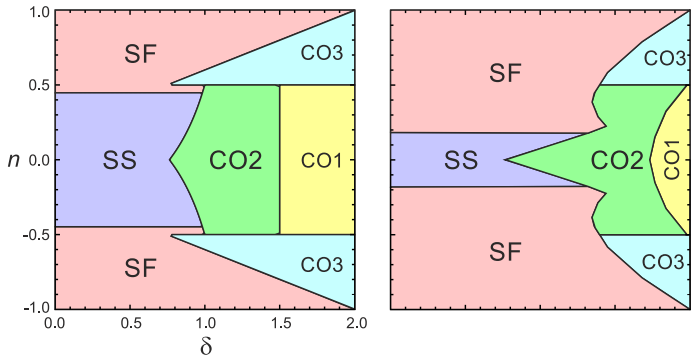

Figure 2: (Color online) The n - δ GS phase diagrams for the model system given $\nu = 0.75$. Left panel shows the MFA results, right panel shows the QMC results.

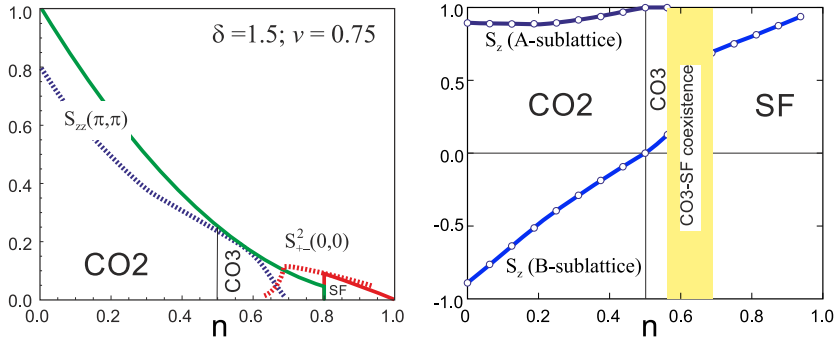

Figure 3: (Color online) Left panel: Correlation functions for the model $S = 1$ pseudospin system given $\delta = 1.5$, $\nu = 0.75$, solid lines are the MFA results, dotted lines are the QMC results. Right panel: QMC data for the sublattice S_z-components as functions of the deviation from the half-filling. Filling points to a CO3-SF coexistence phase typical for the first kind phase transition.

and CO2 phases into the CO3 phase. The line of the first order phase transition CO3-SF in Fig. 2 corresponds to the equality of the respective energies. It is worth to note that the critical concentration n for the SS-SF, CO1-CO3 and CO2-CO3 transitions does not depend on the correlation parameter δ.

In Fig. 3 (top panel, solid lines) we present the n-dependence of the correlation functions $S_{zz}(\pi,\pi) = \langle S_z, S_z\rangle$ (static structure factor) and $S^2_{+-}(0,0) = \langle S^2_+, S^2_-\rangle$ at $\delta = 1.5$, $\nu = 0.75$, determining the long-range CO and SF orders, respectively, given $\delta = 1.5$, that is in an immediate closeness to CO2-CO1 phase transition for small n.

4. Quantum Monte-Carlo calculations

We have performed Quantum Monte-Carlo (QMC) [10] calculations for our model Hamiltonian (1). In Fig. 2 we compare the ground state δ - n phase dia-

gram of our model 2D system calculated on square lattice 12×12 given $\nu = 0.75$ with that of calculated within MFA approach. As for a simple hard-core counterpart [6, 9], despite some qualitative agreement, we see rather large quantitative difference between two diagrams in Fig. 2. In particular, it concerns a clearly larger volume of the quantum SF phase that might be related with a sizeable suppression of quantum fluctuations within MFA approach. The SF-SS transition line does not depend on the correlation parameter δ in MFA calculations as well as in QMC ones since both these phases consist of only the $M = \pm 1$ states having the same dependence of the energy on δ. The location of the CO1-CO3 and CO2-CO3 transition lines at $|n| = 0.5$, both for MFA and QMC, has a trivial structural reason. The filling of the lattice by $M = \pm 1$ centers for CO1 phase or by $M = 0$ centers for CO2 phase during the doping leads on the lines $n = \pm 0.5$ to identical result that minimizes the energy of the inter-site density-density interactions. Namely, this is the initial state of CO3 phase, when the first sublattice is completely filled by $M = 0$ centers and the second one is completely filled by $M = \pm 1$ centers. In contrast to MFA, the CO1-CO2 transition line in QMC calculations shows evident dependence on n that implies a more complicated structure of the CO1 and CO2 phases as compared with MFA. This leads, in particular, to the fact that the triple point of the CO1-CO2-CO3 phases shifts from the MFA values $n = 0.5$, $\delta = 1.5$ to $n = 0.5$, $\delta = 2.0$.

In Fig. 3 (left panel, two dotted lines) we present the QMC calculated static structure factor $S_{zz}(\pi, \pi)$ and the superfluid (pseudospin nematic) correlation function $S^2_{+-}(0, 0)$. It is worth to note a semiquantitative agreement with the MFA data. Smaller value of the quantum structure factor $S_{zz}(\pi, \pi)$ at $n = 0$ is believed to be a result of the pseudospin reduction due to quantum fluctuations. Right panel in Fig. 3 shows the n-dependence of the mean sublattice S_z values, S_{Az} and S_{Bz}, that clearly demonstrates the pseudospin quantum reduction effect within CO2 phase and specific features of the sublattice occupation, or "pseudo-magnetization" under CO2-CO3-SF transformation. Also, note that these QMC data points to the CO3-SF phase coexistence typical for the first kind phase transition, but obviously absent in MFA.

It should be noted that the results of QMC calculations for the system 12×12 presented here vary slightly compared to the system 8×8, that supports their validity. Calculations for larger lattices are in progress.

5. Conclusions

A simplified 2D $S = 1$ pseudospin Hamiltonian with a two-particle transport term (pseudospin nematic coupling) was analyzed within a generalized MFA and QMC technique. We have obtained the ground-state phase diagrams and correlation functions given different values of the coupling parameters with a focus on the role of the on-site correlation effect (single-ion anisotropy). The comparison of the two methods allows us to uncover fundamental shortcomings of the MFA technique and clearly demonstrate the role of quantum effects.

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